

# MOFs for CO<sub>2</sub> Capture and Separation from Flue Gas Mixtures: The Effect of Multifunctional Sites on Their Adsorption Capacity and Selectivity

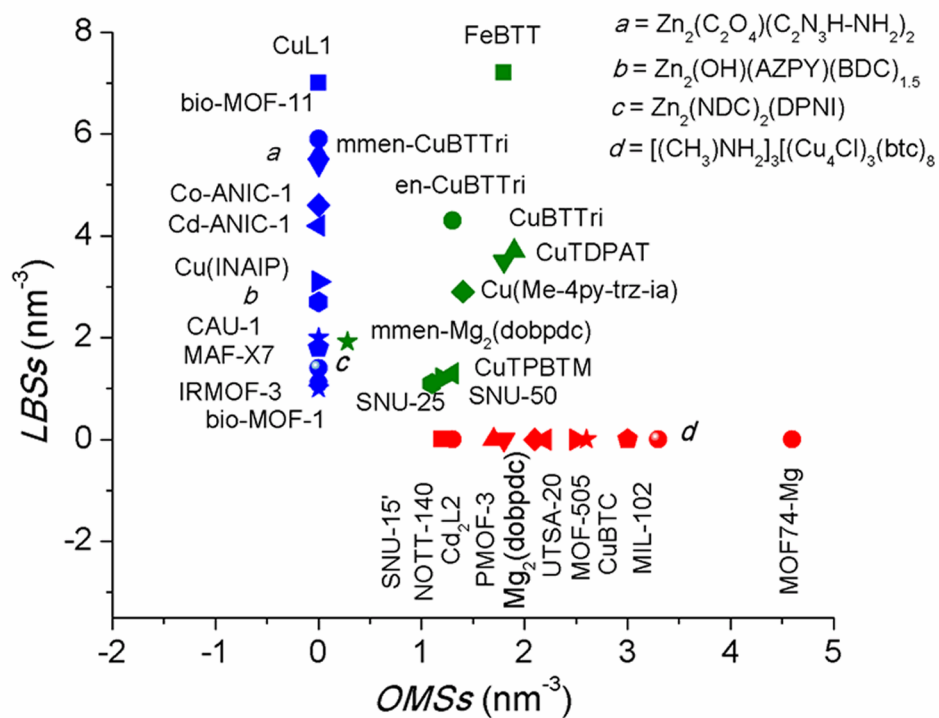
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## Supporting Information



**Fig. S1.** The OMS and LBS density map. Detailed data are listed in Tables 1-4 in the paper. (L1 = 5-(1H-tetrazol-1-yl)isophthalic acid; L2 = 4,4'-(hexafluoroisopropylidene)diphthalate.) (Red points: MOFs with only OMSs; blue points: MOFs with only LBSs; Olive points: MOFs with both OMSs and LBSs).

**Table S1.** Relationship of density of OMSs or LBSs/OFSs with the CO<sub>2</sub> uptake and CO<sub>2</sub>/N<sub>2</sub> selectivity

Compounds	OMSs (nm <sup>-3</sup> )	LBSs/OFSs (nm <sup>-3</sup> )	Qst of CO <sub>2</sub> (kJ/mol)	Selectivity CO <sub>2</sub> :N <sub>2</sub> =15:85	CO <sub>2</sub> uptake (wt%) (0.15 atm)	Ref
m <sup>m</sup> en-CuBTTri	0	5.6	96	327	10.5	1-2
en-CuBTTri	1.3	4.3	90	143	2.3	3
CuBTTri	1.9	3.7	21	17	3.0	3
FeBTT	1.8	7.2		61	5.3	4
MOF-74-Mg	4.6	0	47	150	27.0	2, 5
Cu-TDPAT	1.8	3.5	42.4	88	7.5	6
Cu-TPBTM	1.3	1.3	26.3	21	4.2	7
PCN-61	1.2	0	22	15	2.5	7
Bio-MOF-11	0	1.0	45	36	5.3	8-9
Zn <sub>2</sub> (bdc-OH) <sub>2</sub> (ted)	0	3.14	24.2	4	2.4	10
CuBTC	2.6	0	30	21	3.8	This work
Cu(bpy-1) <sub>2</sub> (SiF <sub>6</sub> )	0	4.02	27	26	3.58	11
Cu(bpy-2) <sub>2</sub> (SiF <sub>6</sub> )	0	1.41	21	23	2.26	11

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